containing 1
fragments assigned reactant/reagent role:
containing 38
node mappings:
19:45 13:40 12:39 14:41 15:42 16:43

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

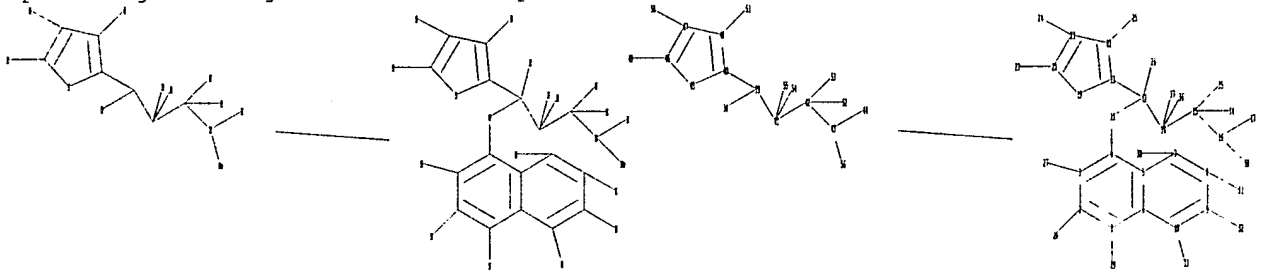
Structure attributes must be viewed using STN Express query preparation.

=> s l3 full
FULL SEARCH INITIATED 13:37:44 FILE 'CASREACT'
SCREENING COMPLETE - 128 REACTIONS TO VERIFY FROM 14 DOCUMENTS

100.0% DONE 128 VERIFIED 1 HIT RXNS (1 INCOMP) 1 DOCS
SEARCH TIME: 00.00.01

L4 1 SEA SSS FUL L3 (1 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\KC3.str

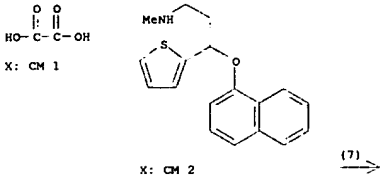


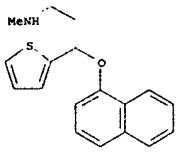
chain nodes :
11 12 14 15 16 17 18 23 24 25 26 27 28 29 30 31 32 33 34 35 36
37 38 39 41 42 43 44 49 50 51 52 53 54 55 56
ring nodes :
1 2 3 4 5 6 7 8 9 10 13 19 20 21 22 40 45 46 47 48

```
chain bonds :
1-29  2-28  3-27  4-11  7-30  8-31  9-32  10-33  11-12  12-13  12-14  12-26  14-15
14-36  14-37  15-16  15-34  15-35  16-17  16-18  20-23  21-24  22-25  38-39  39-40
39-41  41-42  41-54  41-55  42-43  42-52  42-53  43-44  43-56  46-49  47-50  48-51
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  13-19  13-22  19-20  20-21
 21-22  40-45  40-48  45-46  46-47  47-48
exact/norm bonds :
4-11  11-12  15-16  38-39  42-43
exact bonds :
1-29  2-28  3-27  7-30  8-31  9-32  10-33  12-13  12-14  12-26  13-19  13-22  14-15
 14-36  14-37  15-34  15-35  16-17  16-18  19-20  20-21  20-23  21-22  21-24  22-25
 39-40  39-41  40-45  40-48  41-42  41-54  41-55  42-52  42-53  43-44  43-56  45-46
 46-47  46-49  47-48  47-50  48-51
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10
isolated ring systems :
containing 1 : 13 : 40 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:CLASS  12:CLASS  13:Atom  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS
19:Atom  20:Atom  21:Atom  22:Atom  23:CLASS  24:CLASS  25:CLASS  26:CLASS
27:CLASS  28:CLASS  29:CLASS  30:CLASS  31:CLASS  32:CLASS  33:CLASS  34:CLASS
35:CLASS  36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:Atom  41:CLASS  42:CLASS
43:CLASS  44:CLASS  45:Atom  46:Atom  47:Atom  48:Atom  49:CLASS  50:CLASS
51:CLASS  52:CLASS  53:CLASS  54:CLASS  55:CLASS  56:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 38
node mappings:
19:45  13:40  12:39  14:41  15:42  16:43



L5      STRUCTURE UPLOADED

=> s l5 full
FULL SEARCH INITIATED 13:38:34 FILE 'CASREACT'
SCREENING COMPLETE -      128 REACTIONS TO VERIFY FROM       14 DOCUMENTS

100.0% DONE     128 VERIFIED      12 HIT RXNS (     1 INCOMP)       7 DOCS
SEARCH TIME: 00.00.01

L6            7 SEA SSS FUL L5 (    12 REACTIONS)

=> s l6 and oxalate
          2750 OXALATE
L7           0 L6 AND OXALATE

=> d ibib abs hit l6 1-7
```

L6 ANSWER 1 OF 7 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 144:108160 CASREACT
TITLE: Synthesis of Duloxetine hydrochloride
AUTHOR(S): Gao, Li-mei; Zhu, Feng-chang; Song, Dan-qing
CORPORATE SOURCE: Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Xinyao Zazhi (2005), 14(1), 74-76
CODEN: ZXZHA6; ISSN: 1003-3734
PUBLISHER: Zhongguo Xinyao Zazhishe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Duloxetine hydrochloride was prepared from 2-acetylthiophene, dimethylamine hydrochloride and paraformaldehyde via Mannich reaction, reduction, optical resolution, etherification in six steps with overall yield 7%. The structure of Duloxetine was identified by MS, 1H NMR and element anal. A simple, easily controlled and low cost process for the synthesis of Duloxetine is provided.

RX(7) OF 19 ...X ===> AC...





AC

L6 ANSWER 1 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

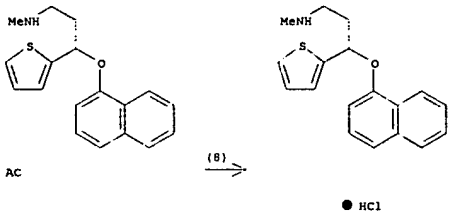
RX(7) RCT X 116817-77-7

STAGE(1)
RGT Y 7664-41-7 NH3
SOL 7732-18-5 Water, 141-78-6 AcOEt

STAGE(2)
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AC 116539-59-4
NTE gas HCl used

RX(8) OF 19 ...AC ===> AD



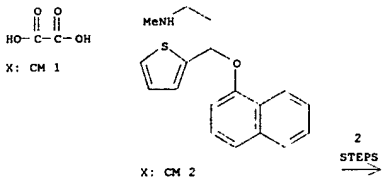
AC

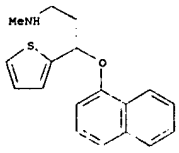
AD

RX(8) RCT AC 116539-59-4
PRO AD 136434-34-9
SOL 67-66-3 CHCl3, 141-78-6 AcOEt
CON overnight, 4 deg C

RX(13) OF 19 COMPOSED OF RX(7), RX(8)
RX(13) X ===> AD

L6 ANSWER 1 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)





HCl

AD

RX(7) RCT X 116817-77-7

STAGE(1)
RGT Y 7664-41-7 NH3
SOL 7732-18-5 Water, 141-78-6 AcOEt

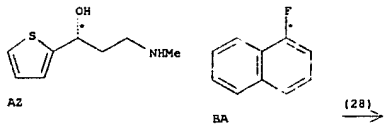
STAGE(2)
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AC 116539-59-4
NTE gas HCl used

RX(8) RCT AC 116539-59-4
PRO AD 136434-34-9
SOL 67-66-3 CHCl3, 141-78-6 AcOEt
CON overnight, 4 deg C

L6 ANSWER 2 OF 7 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 143:133071 CASREACT
TITLE: Polymer-supported chiral sulfonamide catalyzed one-pot reduction of β-keto nitriles: a practical synthesis of (R)-fluoxetine and (R)-duloxetine
AUTHOR(S): Wang, Guangyin; Liu, Xingshun; Zhao, Gang
CORPORATE SOURCE: Laboratory of Modern Synthetic Organic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Tetrahedron: Asymmetry (2005), 16(10), 1873-1879
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Enantioselective reduction of β-keto nitriles to optically active 1,3-amino alcs. has been carried out in one step using an excess of borane-dimethyl sulfide complex as a reductant and a polymer-supported chiral sulfonamide as a catalyst with moderate to high enantioselectivity.
The facile and enantioselective method to prepare optically active 1,3-amino alcs. to be converted into 3-aryloxy-3-arylpropylamine-type antidepressant drugs (R)-fluoxetine, and (R)-duloxetine is also reported.
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

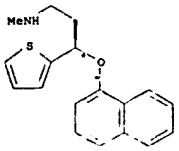
RX(28) OF 48 ...AZ + BA ===> BB



AZ

BA

L6 ANSWER 2 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BB
YIELD 88%

RX(28) RCT AZ 116539-57-2

STAGE(1)
RGT AW 7646-69-7 NaH
SOL 67-68-5 DMSO
CON 30 minutes, room temperature

STAGE(2)
RCT BA 321-38-0
CON 1 hour, 40 - 50 deg C

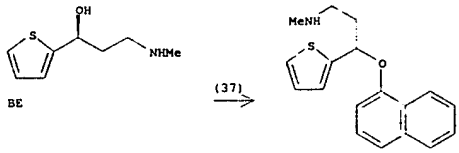
PRO BB 116539-60-7

L6 ANSWER 3 OF 7 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 142:481782 CASREACT
TITLE: Practical synthesis of enantiopure γ-amino alcohols by rhodium-catalyzed asymmetric hydrogenation of β-secondary-amino ketones
AUTHOR(S): Liu, Duan; Gao, Wenzhong; Wang, Chunjiang; Zhang, Xumu
CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Angewandte Chemie, International Edition (2005), 44(11), 1687-1689
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several β-secondary amino ketone hydrochlorides were hydrogenated with remarkably high enantioselectivities by using a rhodium complex containing P-chiral bisphospholane. These results establish a short and practical means for the synthesis of enantiopure N-monosubstituted γ-amino alcs., which are key intermediates in the synthesis of important antidepressants. For example, the bis[di(methyl)ethyl]tetra(hydro)-1,1'-bi-1H-isophosphindole-rhodium-catalyzed stereoselective hydrogenation of 3-(methylamino)-1-phenyl-1-propanone hydrochloride gave (αS)-α-[2-[(methyl)amino]ethyl]benzenemethanol, which is a synthetic precursor for (γS)-N-methyl-γ-[4-(trifluoromethyl)phenoxy]benzenepropanamine (i.e., (S)-fluoxetine]. The synthesis of (αS)-[-[(methyl)amino]ethyl]thiophenemethanol, a key synthetic intermediate for (S)-duloxetine, was also reported.

VERIFICATION INCOMPLETE - REACTION MAP DATA UNAVAILABLE

RX(37) OF 74 ...BE ===> BJ

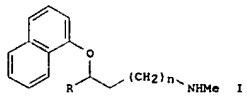


BE BJ

RX(37) RCT BE 116539-55-0
PRO BJ 116539-59-4
NTE literature preparation

L6 ANSWER 3 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

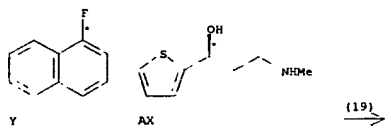
L6 ANSWER 4 OF 7 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:145879 CASREACT
TITLE: Duloxetine (Cymbalta), a dual inhibitor of serotonin and norepinephrine reuptake
AUTHOR(S): Bymaster, F. P.; Beedle, E. E.; Findlay, J.; Gallagher, P. T.; Krushinski, J. H.; Mitchell, S.; Robertson, D. W.; Thompson, D. C.; Wallace, L.; Wong, D. T.
CORPORATE SOURCE: Eli Lilly and Company, Lilly Research Laboratories, Lilly Corporate Center, Indianapolis, IN, 46285, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(24), 4477-4480
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

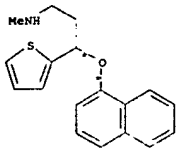
AB A series of naphthalenyloxy-substituted amines I (n = 2 - 4, R = H; n = 1, R = H, Ph, 4-FC6H4, 2-MeOC6H4, 2-furyl, 2-thienyl, 2-thiazolyl, etc.) has been prepared, and these compds. are demonstrated to be inhibitors of both serotonin and norepinephrine reuptake. One member of this series, duloxetine (Cymbalta), (S)-I (n = 1; R = 2-thienyl), has proven to be effective in clin. trials for the treatment of depression.
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(19) OF 32 ...Y + AX ===> BE



Y AX

L6 ANSWER 4 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



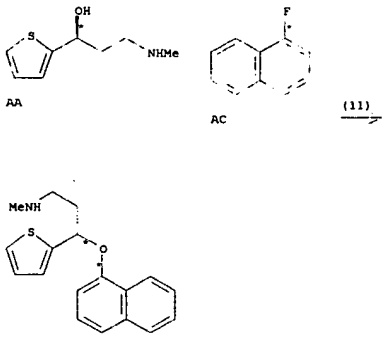
BE

RX(19) RCT Y 321-38-0, AX 116539-55-0
RGT D 7646-69-7 NaH
PRO BE 116539-59-4
SOL 127-19-5 AcNMe2

L6 ANSWER 5 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 139:245838 CASREACT
TITLE: Chemoenzymatic synthesis of duloxetine and its enantiomer: lipase-catalyzed resolution of 3-hydroxy-3-(2-thienyl) propanenitrile
AUTHOR(S): Kamal, Ahmed; Khanna, G. B. Ramesh; Ramu, R.; Krishnaji, T.
CORPORATE SOURCE: Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SOURCE: Tetrahedron Letters (2003), 44(25), 4783-4787 CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An efficient and facile chemoenzymic synthesis of duloxetine by lipase-mediated resolution of 3-hydroxy-3-(2-thienyl)propanenitrile has been achieved. This process also describes an enantioconvergent synthesis of duloxetine via a Mitsunobu reaction.
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(11) OF 89 ...AA + AC ===> AD



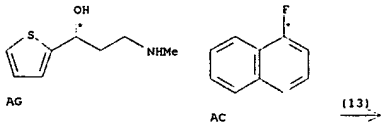
AA AC (11)

AD
YIELD 81%

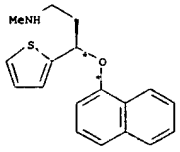
L6 ANSWER 5 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(11) RCT AA 116539-55-0, AC 321-38-0
RGT AE 7646-69-7 NaH
PRO AD 116539-59-4
SOL 67-68-5 DMSO
CON 8 hours, room temperature

RX(13) OF 89 ...AG + AC ===> AH



AG AC (13)

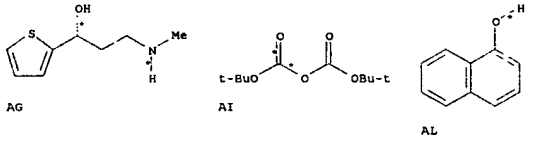


AH
YIELD 81%

RX(13) RCT AG 116539-57-2, AC 321-38-0
RGT AE 7646-69-7 NaH
PRO AH 116539-60-7
SOL 67-68-5 DMSO
CON 8 hours, room temperature

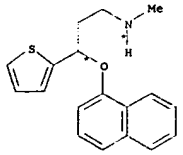
RX(61) OF 89 COMPOSED OF RX(14), RX(15), RX(16)
RX(61) AG + AI + AL ===> AD

L6 ANSWER 5 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AG AI AL

3 STEPS

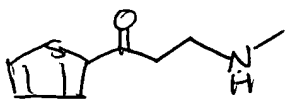


AD
YIELD 70%

RX(14) RCT AG 116539-57-2, AI 24424-99-5
RGT AK 121-44-8 Et3N
PRO AJ 597581-31-2
SOL 75-09-2 CH2Cl2
CON 2 hours, room temperature

RX(15) RCT AJ 597581-31-2, AL 90-15-3
RGT AN 603-35-0 PPh3, AO 2446-83-5 N2(CO2CHMe2)2
PRO AM 597581-32-3
SOL 109-99-9 THF
CON 24 hours, room temperature
NTE Mitsunobu reaction, stereoselective

RX(16) RCT AM 597581-32-3
RGT AP 76-05-1 F3CCO2H
PRO AD 116539-59-4
SOL 67-66-3 CHCl3

Prep of Duloxetine Duloxetin from 

10/542003

~~10/490,546~~

10/06/2006

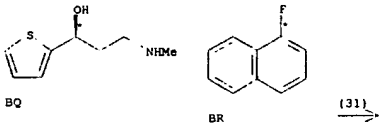
L6 ANSWER 6 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 139:84781 CASREACT
TITLE: Enantioselective hydrogenation of β-keto esters using chiral diphosphine-ruthenium complexes: Optimization for academic and industrial purposes and synthetic applications
AUTHOR(S): Ratovelomanana-Vidal, V.; Girard, C.; Touati, R.; Tranchier, J. P.; Ben Hassine, B.; Genet, J. P.
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels (UMR 7573 CNRS), Ecole Nationale Superieure de Chimie de Paris, Paris, 75005, Fr.
SOURCE: Advanced Synthesis & Catalysis (2003), 345(1+2), 261-274
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Enantioselective hydrogenation using chiral complexes between atropisomeric diphosphines and ruthenium is a powerful tool for producing chiral compds. Using a simple and straightforward in situ catalyst preparation, the conditions were optimized using mol. hydrogen. This led to the best conditions and the lowest catalytic ratio required for the pressure used. Hydrogenation of various β-keto esters was efficiently performed at atmospheric and higher pressures, leading to the use of very low catalyst-substrate ratios up to 1/20,000. Asym. hydrogenations were used in key-steps towards the total synthesis of corynomycolic acid, Duloxetine and Fluoxetine.

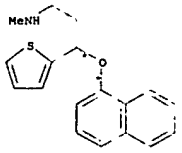
REFERENCE COUNT: 119 THERE ARE 119 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(31) OF 82 ...BQ + BR ===> BS



BQ BR (31)

L6 ANSWER 6 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BS
YIELD 62%

RX(31) RCT BQ 116539-55-0

STAGE(1)
RGT AM 7646-69-7 NaH
SOL 127-19-5 AcNMe2
CON 1.5 hours, 50 deg C

STAGE(2)
RCT BR 321-38-0
CON 2.5 hours, 80 deg C

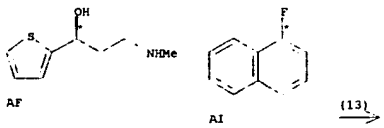
PRO BS 116539-59-4

L6 ANSWER 7 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 123:55626 CASREACT
TITLE: An asymmetric synthesis of duloxetine hydrochloride, a mixed uptake inhibitor of serotonin and norepinephrine, and its C-14 labeled isotopomers
AUTHOR(S): Wheeler, William J.; Kuo, Fengjiun
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly Co., Indianapolis, IN, 46285, USA
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1995), 36(3), 213-23
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

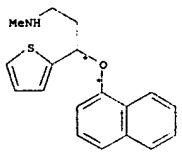
AB Two 14C-isotopomers of duloxetine HCl [S-(+)-N-methyl-γ-(1-naphthalenyloxy)-2-thiophenepropanamine hydrochloride] have been prepared by an asym. synthesis. The palladium catalyzed cross-coupling of 2-thienoyl chloride (or its [carbonyl-14C] isotopomer) with vinyltributylstannane, followed by addition of HCl afforded the key pro-chiral intermediate chloro ketone. Chiral reduction with borane in the presence of the appropriate oxazaborolidine catalyst provided the S-chloro alc. and its 14C-labeled counterpart or the analogous R-chloro alc. Activation of the chloro alcs. by reaction with NaI/acetone, followed by reaction of the corresponding iodo alcs. with methylamine yielded the penultimate amino alcs. Formation of the alkoxide with NaH, followed by reaction with 1-fluoronaphthalene yielded duloxetine or its 14C-labeled isotopomer. Alternatively, reaction of the R-chloro alc. with 1-naphthol-[1-14C] under Mitsunobu conditions afforded a aryl ether, which was in turn activated by reaction with NaI/acetone. Subsequent reaction with methylamine followed by salt formation yielded duloxetine or its naphthalene-labeled isotopomer as their HCl salts.

RX(13) OF 75 ...AF + AI ===> AJ



AF AI (13)

L6 ANSWER 7 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● HCl

AJ
YIELD 45%

RX(13) RCT AF 116539-55-0

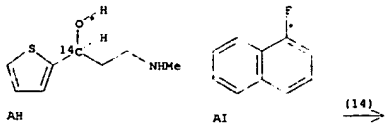
STAGE(1)
RGT AK 7646-69-7 NaH
SOL 127-19-5 AcNMe2

STAGE(2)
RCT AI 321-38-0

STAGE(3)
RGT Q 7647-01-0 HCl
SOL 141-78-6 AcOEt

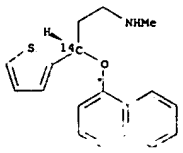
PRO AJ 136434-34-9

RX(14) OF 75 ...AH + AI ===> AN



AH AI (14)

L6 ANSWER 7 OF 7 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● HCl

AN
YIELD 67%

RX(14) RCT AH 164071-60-7

STAGE(1)
RGT AK 7646-69-7 NaH
SOL 127-19-5 AcNMe2

STAGE(2)
RCT AI 321-38-0

STAGE(3)
RGT Q 7647-01-0 HCl
SOL 141-78-6 AcOEt

PRO AN 164071-51-6

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=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    387.00     387.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     -4.97      -4.97

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DICTIONARY FILE UPDATES:    5 OCT 2006  HIGHEST RN 909768-05-4

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=> s  116817-77-7/rn
L8            1 116817-77-7/RN   <-oxalate

=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                      0.44     387.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                      0.00      -4.97

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FILE LAST UPDATED: 5 Oct 2006 (20061005/ED)

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=> s l8
L9 9 L8

=> d ibib abs hit 1-9

L9 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1061536 CAPLUS
DOCUMENT NUMBER: 143:416025
TITLE: Chronic treatment with duloxetine is necessary for an anxiolytic-like response in the mouse zero maze: the role of the serotonin transporter
AUTHOR(S): Troelsen, K. B.; Nielsen, E. O.; Mirza, N. R.
CORPORATE SOURCE: NeuroSearch A/S, Ballerup, 2750, Den.
SOURCE: Psychopharmacology (Berlin, Germany) (2005), 181(4), 741-750
CODEN: PSCHDL; ISSN: 0033-3158
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Monoamine transporter inhibitor antidepressants have anxiolytic efficacy in man. However, preclin. data poorly reflect this, either because (1) few studies assess chronic antidepressant treatment in animal models, (2) antidepressants are anxiogenic after acute treatment; and (3) animal models of anxiety are insensitive to antidepressants. We address issues (1) and (2) and ascertain potential mechanisms mediating anxiolytic effects demonstrated. The effect of acute treatment with seven antidepressants covering the classes selective serotonin reuptake inhibitors, serotonin-noradrenaline reuptake inhibitors, noradrenaline reuptake inhibitors and tricyclic antidepressants were compared with the benzodiazepine, chlordiazepoxide, on the mouse zero maze, an unconditioned model of anxiety. Furthermore, citalopram, duloxetine, reboxetine and amitriptyline were assessed after chronic administration (10 mg/kg p.o., 21 days, twice daily) in this model. In mice treated chronically, (a) the hypothermic response to serotonin (5-HT)1A and 5-HT1B receptor ligands, 8-hydroxy-2-(die-n-propylamino)tetralin (8-OHDPAT) and m-chlorophenyl piperazine (mCPP), resp., was assessed and (b) serotonin transporter (SERT) and noradrenaline transporter (NET) densities in the cortex and hippocampus, resp., were determined None of the antidepressants were anxiolytic after acute treatment, although reboxetine, duloxetine and amitriptyline were anxiogenic. Only chronic treatment with duloxetine induced an anxiolytic effect, which was dissociable from nonspecific motor effects. Duloxetine reduced SERT d. in the cortex by .apprx.75% compared to control, with no effect on NET d. in the hippocampus. Citalopram and amitriptyline significantly reduced SERT d. by .apprx.20%, whereas reboxetine selectively reduced NET d. All drugs reduced the hypothermic response to 8-OHDPAT and mCPP. Duloxetine was anxiolytic after chronic but not acute treatment, reflecting clin. experience with antidepressants in general. Duloxetine's anxiolytic-like profile may be ascribed to the considerable reduction in the d. of the SERT in the cortex.
REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
IT 549-18-8, Amitriptyline hydrochloride 12794-10-4, Benzodiazepine 56296-78-7, Fluoxetine hydrochloride 59729-32-7, Citalopram hydrobromide 78246-49-8, Paroxetine hydrochloride 99300-78-4, Venlafaxine hydrochloride 116817-77-7, Duloxetine oxalate 868161-64-2, Reboxetine fumarate
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(role of SERT in anxiolytic response to chronic duloxetine in mice)

L9 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:250010 CAPLUS
DOCUMENT NUMBER: 144:108160
TITLE: Synthesis of Duloxetine hydrochloride
AUTHOR(S): Gao, Li-mei; Zhu, Feng-chang; Song, Dan-qing
CORPORATE SOURCE: Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Zhongguo Xinyao Zazhi (2005), 14(1), 74-76
CODEN: ZXZHA6; ISSN: 1003-3734
PUBLISHER: Zhongguo Xinyao Zazhishe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 144:108160
AB Duloxetine hydrochloride was prepared from 2-acetylthiophene, dimethylamine hydrochloride and paraformaldehyde via Mannich reaction, reduction, optical resolution, etherification in six steps with overall yield 7%. The structure of Duloxetine was identified by MS, 1H NMR and element anal. A simple, easily controlled and low cost process for the synthesis of Duloxetine is provided.
IT 5424-47-5P 13636-02-7P 116539-59-4P 116817-77-7P 132335-47-8P 287737-72-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of Duloxetine hydrochloride)

L9 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:605494 CAPLUS
DOCUMENT NUMBER: 141:140312
TITLE: 3-Methylamino-1-(2-thienyl)-1-propanone preparation and its use as a pharmaceutical intermediate
PATENT ASSIGNEE(S): BASF Ag, Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10302595	A1	20040729	DE 2003-10302595	20030122
CA 2513542	AA	20040805	CA 2004-2513542	20040115
WO 2004065376	A1	20040805	WO 2004-EP237	20040115
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ				
EP 1587802	A1	20051026	EP 2004-702333	20040115
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1742003	A	20060301	CN 2004-80002686	20040115
JP 2006515878	T2	20060608	JP 2006-500570	20040115
US 2006128791	A1	20060615	US 2005-542003	20050712

PRIORITY APPLN. INFO.: DE 2003-10302595 A 20030122
WO 2004-EP237 W 20040115

AB 3-Methylamino-1-(2-thienyl)-1-propanone and its acid addition salts (e.g., the hydrochloride), which are useful as an intermediate in the production of the pharmaceutical (+)-(S)-N-methyl-3-(1-naphthyloxy)-3-(2-thienyl)propylamine oxalate (i.e., Duloxetine oxalate), are prepared
IT 116539-59-4P, Duloxetine 116817-77-7P, Duloxetine oxalate
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of)

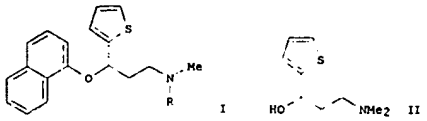
L9 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:546493 CAPLUS
DOCUMENT NUMBER: 141:106360
TITLE: A process of preparation of (+)-duloxetine
INVENTOR(S): Rao, Dharmaraj Ramachandra; Kankan, Rajendra Narayanrao; Wain, Christopher Paul
PATENT ASSIGNEE(S): Cipla Ltd, India
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056795	A1	20040708	WO 2003-GB5357	20031210
WO 2004056795	C1	20050811		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2510750	AA	20040708	CA 2003-2510750	20031210
AU 2003292396	A1	20040714	AU 2003-292396	20031210
BR 2003016902	A	20051025	BR 2003-16902	20031210
EP 1587801	A1	20051026	EP 2003-767973	20031210
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1747947	A	20060315	CN 2003-80109793	20031210
JP 2006514030	T2	20060427	JP 2004-561607	20031210
EP 1690861	A2	20060816	EP 2006-75798	20031210
EP 1690861	A3	20060906		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LV, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
US 2006205956	A1	20060914	US 2006-539415	20060320

PRIORITY APPLN. INFO.: GB 2002-29583 A 20021219
EP 2003-767973 A3 20031210
WO 2003-GB5357 W 20031210

OTHER SOURCE(S): CASREACT 141:106360; MARPAT 141:106360
GI

L9 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB The invention relates to a process for preparing (+)-duloxetine (I), or an acid addition salt thereof, which comprises (a) resolving racemic (±)-duloxetine with a chiral acid so as to obtain a salt of the chiral acid and (+)-duloxetine, substantially free of (-)-duloxetine; and (b) if desired, converting the salt prepared in step (a) to the free base or another acid addition salt as appropriate. The process for preparing (+)-duloxetine, or an acid addition salt thereof, can further comprise an O-alkylation intermediate process step which is carried out in the presence of a base and a phase transfer catalyst. For instance, (S)-duloxetine hydrochloride (I•HCl, R = H) was prepared via etherification of alc. II by 1-fluoronaphthalene in the presence of 18-crown-6, and subsequent N-demethylation of the obtained oxalate salt of I (R = Me) (example 4 and 5).
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
IT 116817-77-7P
RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(process of preparation of (+)-duloxetine via resolution of (±)-duloxetine)

L9 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:856227 CAPLUS
DOCUMENT NUMBER: 135:70315
TITLE: Duloxetine oxalate: Treatment of stress urinary incontinence, antidepressant norepinephrine reuptake inhibitor, 5-HT reuptake inhibitor
AUTHOR(S): Sorbera, L. A.; Castaner, R. M.; Castaner, J.
CORPORATE SOURCE: Prous Science, Barcelona, 08080, Spain
SOURCE: Drugs of the Future (2000), 25(9), 907-916
CODEN: DRFUD4; ISSN: 0377-8282
PUBLISHER: Prous Science
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 48 refs. Topics discussed include: synthesis, pharmacol. actions, pharmacokinetics, clin. studies of duloxetine oxalate.
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
IT 116817-77-7, Duloxetine oxalate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(antidepressant, norepinephrine reuptake inhibitor, 5-HT reuptake inhibitor duloxetine oxalate in treatment of stress urinary incontinence)

L9 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:630192 CAPLUS
DOCUMENT NUMBER: 123:40949
TITLE: Pharmaceutical compositions containing venlafaxine or aryloxy propanamine derivatives for treatment of incontinence
INVENTOR(S): Thor, Karl Bruce
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 654264	A1	19950524	EP 1994-308604	19941122
EP 654264	B1	20010530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CA 2136120	AA	19950525	CA 1994-2136120	19941118
ZA 9409190	A	19960520	ZA 1994-9190	19941118
NO 9404456	A	19950526	NO 1994-4456	19941121
NO 313535	B1	20021021		
IL 111705	A1	20010111	IL 1994-111705	19941121
AU 9478968	A1	19950601	AU 1994-78968	19941122
AU 679269	B2	19970626		
JP 07188003	A2	19950725	JP 1994-288119	19941122
JP 3681009	B2	20050810		
ES 2157958	T3	20010901	ES 1994-308604	19941122
PT 654264	T	20010928	PT 1994-308604	19941122
CN 1107699	A	19950906	CN 1994-118993	19941123
CN 1099284	B	20030122		
HU 72317	A2	19960429	HU 1994-3369	19941123
HU 218920	B	20001228		
RU 2152786	C2	20000720	RU 1994-41950	19941123
CZ 289069	B6	20011017	CZ 1994-2893	19941123
US 5744474	A	19980428	US 1995-425703	19950420
HK 1013799	A1	20020208	HK 1998-115196	19981223
CZ 290573	B6	20020814	CZ 2001-1091	20010323
GR 3036446	T3	20011130	GR 2001-401296	20010827

PRIORITY APPLN. INFO.: US 1993-158121 A 19931124
CZ 1994-2893 A3 19941123

OTHER SOURCE(S): MARPAT 123:40949
AB Urinary incontinence in humans is treated by administration of venlafaxine or a compound chosen from a series of aryloxy propanamines (Markush structure given). Thus, 13.5 g of (S)-(-)-N,N-dimethyl-3-hydroxy-3-(2-ethienyl)propanamine (preparation given) in dimethylsulfoxide was reacted with 12.8 g 1-fluoronaphthalene and stirred for 2.5 h at 60-65° to obtain (S)-(+)-N,N-dimethyl-3-(naphthalenyloxy)-3-(2-ethienyl)propanamine (I). I was dissolved in 14% EtOH (10mg/mL) and diluted with saline to allow appropriate dose injection in a volume of 0.1-0.3 mL/kg i.v. to cats. I produced dose-dependent increase in bladder capacity, to about 5 times the capacity seen under control conditions. A capsule contained I.HCl 5,

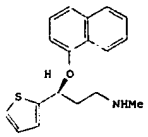
L9 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
starch 445, and Mg stearate 10 mg.
IT 93413-69-5P, Venlafaxine 116817-77-7P 132335-44-5P
136434-34-9P 164015-33-2P 164015-34-3P 164015-36-5P 164015-37-6P
164015-38-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(pharmaceutical compns. containing venlafaxine or aryloxy propanamine
derivs. for treatment of incontinence)

L9 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:106081 CAPLUS
DOCUMENT NUMBER: 116:106081
TITLE: Chiral synthesis of 1-aryl-3-aminopropan-1-ols
INVENTOR(S): Staszak, Michael Alexander; Staten, Gilbert Stanley; Weigel, Leland Otto
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 457559	A2	19911121	EP 1991-304345	19910515
EP 457559	A3	19930512		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
CA 2042346	AA	19911118	CA 1991-2042346	19910510
FI 9102280	A	19911118	FI 1991-2280	19910510
HU 57760	A2	19911230	HU 1991-1648	19910516
JP 04226948	A2	19920817	JP 1991-113034	19910517
PRIORITY APPLN. INFO.:			US 1990-524512 A	19900517

OTHER SOURCE(S): CASREACT 116:106081; MARPAT 116:106081
AB RCH(OH)CH2CH2NR1R2 (I; R = Ph, thienyl; R1, R2 = alkyl, phenylalkyl) were prepd by reduction of the corresponding ketones with a complex of LiAlH4 with (2R,3S)-(-)-4-(dimethylamino)-3-methyl-1,2-diphenyl-2-butanol. Thus, 3-(dimethylamino)-1-(2-thienyl)-1-propanone hydrochloride was neutralized with NaOH, and the free base was treated with the above complex in toluene to give I (R = 2-thienyl, R1 = R2 = Me) (85.8% (-)-isomer and 14.2% (+)-isomer). The (-)-isomer was isolated in 98.7% purity.
IT 5554-64-3P 116539-59-4P 116817-77-7P 116817-78-8P
116817-86-8P 132335-46-7P 132335-49-0P 138760-50-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:121917 CAPLUS
DOCUMENT NUMBER: 114:121917
TITLE: Asymmetric synthesis and absolute stereochemistry of LY248686
AUTHOR(S): Deeter, Jack; Frazier, Jeff; Staten, Gilbert; Staszak, Mike; Weigel, Leland
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly and Co., Indianapolis, IN, 46285, USA
SOURCE: Tetrahedron Letters (1990), 31(49), 7101-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:121917
GI



I

AB Reduction of 3-(dialkylamino)-1-aryl-1-propanones with a 2:1 complex of (2R,3S)-PhCH2CPh(OH)CHMeCH2NMe2 and LiAlH4 provided the corresponding 1,3-amino alcs. in high enantiomeric excesses (80-88%). This process was developed and applied to the synthesis of LY248686 (I), a potent inhibitor of serotonin and norepinephrine uptake. Absolute configurations have been established by single crystal x-ray anal.
IT 40116-79-8P 116817-77-7P 116817-86-8P 132335-49-0P
132335-50-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:570224 CAPLUS
DOCUMENT NUMBER: 109:170224
TITLE: Preparation of 3-aryloxy-3-substituted-propanamines as antidepressants
INVENTOR(S): Robertson, David Wayne; Wong, David Taiwai; Krushinski, Joseph Herman, Jr.
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
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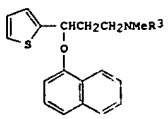
EP 273658	A1	19880706	EP 1987-311181	19871218
EP 273658	B1	19901031		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 8782660	A1	19880623	AU 1987-82660	19871217
AU 591007	B2	19891123		
DK 8706648	A	19880623	DK 1987-6648	19871217
DK 174599	B1	20030714		
ZA 8709472	A	19890830	ZA 1987-9472	19871217
SU 1598865	A3	19901007	SU 1987-4203804	19871217
IL 84863	A1	19920329	IL 1987-84863	19871217
CA 1302421	A1	19920602	CA 1987-554601	19871217
CN 87108175	A	19880706	CN 1987-108175	19871218
CN 1019113	B	19921118		
JP 63185946	A2	19880801	JP 1987-322617	19871218
JP 2549681	B2	19961030		
HU 47561	A2	19890328	HU 1987-5863	19871218
HU 206309	B	19921028		
AT 57924	E	19901115	AT 1987-311181	19871218
US 4956388	A	19900911	US 1990-462925	19900112
US 5023269	A	19910611	US 1990-499940	19900327
PRIORITY APPLN. INFO.:			US 1986-945122 A	19861222
			EP 1987-311181 A	19871218
			US 1990-462925 A3	19900112

OTHER SOURCE(S): MARPAT 109:170224
GI



II

AB R1CH(OAr)CH2CH2NR2R3 (I) (Ar = Ph, naphthyl, mono- or dihalo-, -alkyl-,

L9 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
-alkoxy-, -CF3-substituted Ph, halo-, alkyl-, or CF3-substituted naphthyl;
R1 = cycloalkyl, furanyl, pyridyl, thiazolyl, thienyl, halothienyl, alkylthienyl; R2,R3 = H, Me) were prepd. 2-Acetylthiophene, Me2NH·HCl, paraformaldehyde, and aq. HCl were refluxed 1.5 h and the product stirred overnight with NaBH4 in aq. MeOH contg. NaOH to give RCH(OH)CH2CH2NMe2 (R = 2-thienyl) which was heated 20 min at 70° with NaH in AcNMe2 followed by addn. of 1-fluoronaphthalene and addnl. 60 min heating at 110° to give naphthalenyloxypropanamine II (R3 = Me). The latter was refluxed 1.5 h in PhMe with ClCO2Ph to give II (R3 = CO2Ph) which was heated 75 min at 110° in MeCH(OH)CH2OH contg. aq. NaOH to give II (R3 = H) (III). (+)-III·(CO2H)2 had IC50 of 12.3 and 38 nM for rat synaptosomal uptake of serotonin and norepinephrine, resp., in vitro. Capsules were prepd. each contg. (+)-III-maleate 250, starch 200, and Mg stearate 10 mg.

IT 116817-11-9P 116817-12-0P 116817-13-1P 116817-14-2P 116817-15-3P
116817-16-4P 116817-17-5P 116817-18-6P 116817-19-7P 116817-20-0P
116817-22-2P 116817-24-4P 116817-26-6P 116817-28-8P 116817-29-9P
116817-30-2P 116817-31-3P 116817-32-4P 116817-34-6P 116817-35-7P
116817-36-8P 116817-38-0P 116817-40-4P 116817-41-5P 116817-42-6P
116817-44-8P 116817-46-0P 116817-48-2P 116817-50-6P 116817-52-8P
116817-54-0P 116817-56-2P 116817-58-4P 116817-60-8P 116817-62-0P
116817-64-2P 116817-66-4P 116817-68-6P 116817-70-0P 116817-72-2P
116817-74-4P 116817-76-6P 116817-77-7P 116817-78-8P
116846-81-2P 117699-22-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antidepressant)

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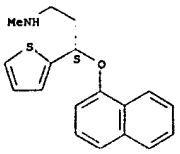
IT 116817-77-7, Duloxetine oxalate
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(role of SERT in anxiolytic response to chronic duloxetine in mice)
RN 116817-77-7 CAPLUS
CN 2-Thiophenepropanamine, N-methyl-γ-(1-naphthalenyloxy)-, (γS)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-59-4
CMF C18 H19 N O S

Absolute stereochemistry. Rotation (+).



CM 2

CRN 144-62-7
CMF C2 H2 O4